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Modeling Inertial Focusing in Straight and Curved Microfluidic Channels

Researchers from Massachusetts General Hospital and Veryst are using multiphysics analysis to investigate the microfluidic process of inertial focusing.

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In many medical procedures and tests it is necessary to isolate cells of interest for further analysis. Microfluidics has revolutionized the way in which these tests are conducted. One of the most promising microfluidic techniques to separate and concentrate cells of interest is called inertial focusing. Originally discovered in the 1960s, the phenomenon of inertial focusing found new utility in microfluidics, and in particular biomedical device design, recently playing a key role in a device enabling the ability to detect cancer from a blood sample. The phenomenon is characterized by suspended particles in a flow spontaneously migrating across streamlines to equilibrium positions within a channel cross-section, where they continue to flow in an ordered formation. By changing the geometry of the channel it is possible to control the equilibrium positions of particles of different sizes.

This phenomenon occurs when the particle Reynolds number, ReP, is approximately equal to 1 and is due to the balance of two forces; a shear gradient lift force directed towards the walls of the channel and a wall-interaction force directed away from each wall. The balance of these two forces determines the equilibrium position (see Figure 1). In a straight channel with a rectangular cross-section this leads to a pair of equilibria centered on the long faces of the channel as shown in Figure 2A. The addition of curvature to the channel changes the resulting force on the particles thus altering the equilibrium positions. A secondary transverse flow occurs across the channel due to the momentum of the faster moving fluid in the center of the channel, which induces a drag force on the particles and thus adjusts their equilibrium positions, as depicted in Figure 2B. The strength of this secondary flow depends on the curvature of the channel and is characterized by the non-dimensional Dean number, De. The equilibrium positions for a particle in curved channel flows are consequently a function of the channel dimensions, particle size, particle and channel Reynolds numbers, and Dean number.

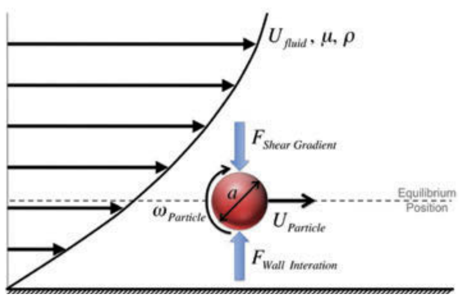

FIGURE 1: Basic forces acting on a particle in a microchannel.

The CFD Model

We developed CFD models in COMSOL Multiphysics to predict the equilibrium locations of the particles and their variation with flow and geometry parameters. To simplify the model and reduce solution time the analysis was divided into two steps. In the first step, we solve a CFD problem that does not include the particle. This gives the standard Hagen-Poiseuille flow solution for straight channels and the Dean flow solution for curved channels. We then map this solution to the inlet boundary of a second CFD model with the particle represented as a void in the CFD domain, with appropriate moving wall conditions to account for the translation and rotation of the particle. Both CFD models were parameterized to facilitate the investigation of the effect of flow and geometry parameters.

The reaction forces and moments on the particle are calculated from the CFD solution and are used to update the particle's translational and rotational velocity components. To accomplish this, we set up global ordinary differential equations (ODEs) specifying the equilibrium of the particle in terms of its linear and angular velocities.

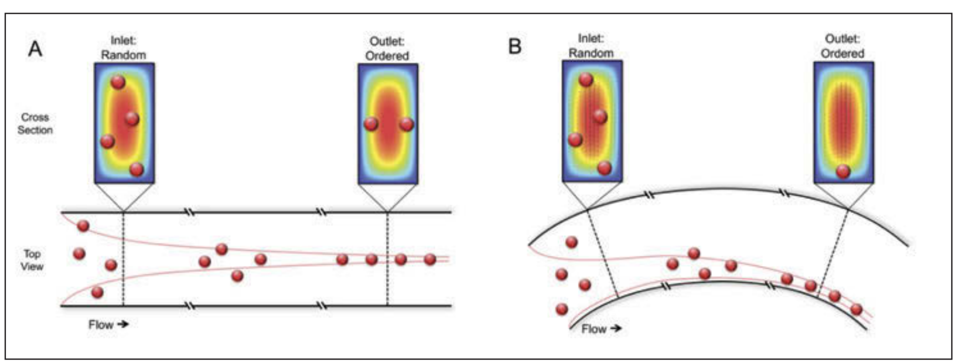

FIGURE 2: Effect of inertial focusing in straight (A) and curved (B) channels. Particles are randomly introduced but become ordered due to inertial focusing, as shown in the cross-section images.

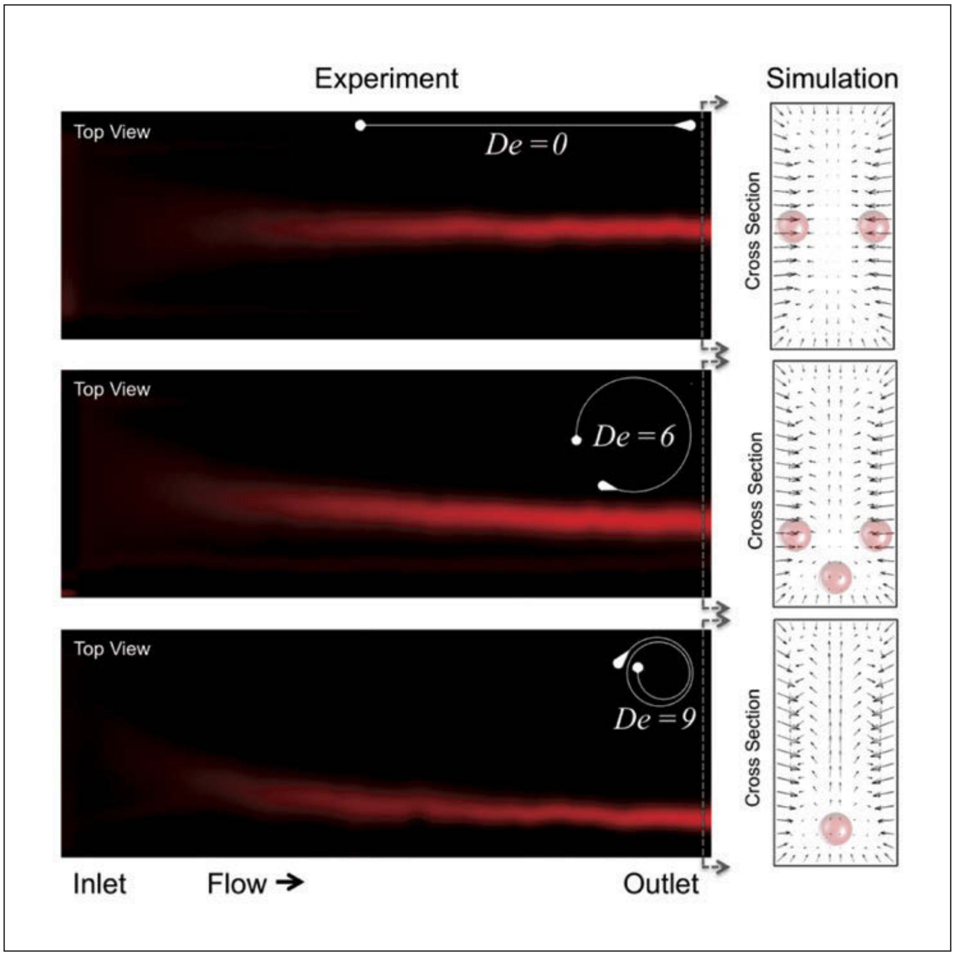

FIGURE 3: Experimental fluorescent microscope images (left) of the longitudinal section of the microchannels showing the distribution of particles along the channel. The cross-section plots (right) show the simulated resultant forces on the particles. The simulated equilibrium positions are marked by the particles and they closely match the experimental results. The data is shown for the same Reynolds number in three microfluidic devices of different curvatures. The curvature of the device is indicated in the inset seen in the upper right corner of the fluorescent images.

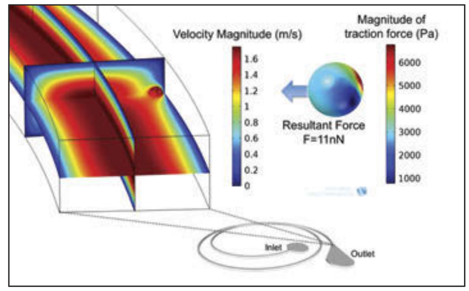

FIGURE 4: Velocity profiles (left) and surface tractions (right) on a particle at a specific non-equilibrium position.

COMSOL Multiphysics solves these global equations simultaneously with the fluid dynamics equations, which significantly speeds up the solution process. Solution time is also improved via the COMSOL Multiphysics unique capability to automatically evaluate the coupling terms between the fluid variables and the global variables in the Jacobian matrix.

After finding the rotational and translational velocities of the particle that are in equilibrium with the surrounding fluid, the transverse inertial lift forces are calculated. We can then add the effect of the Dean flow, assuming Stokes drag on a particle and the Dean flow velocities obtained in the first model.

It is important to recognize that the solution approach described here is required in order to predict inertial focusing since standard particle tracing is not applicable. In a straight channel, for example, standard particle tracing will predict that a neutrally buoyant particle inserted at a specific location in the channel cross-section will remain at that location. There are no general analytical equations relating the forces and moments that govern inertial focusing to the fluid flow conditions obtained in the absence of the particle. We are, however, developing expressions for the forces and moments acting on particles based on the above CFD solution. We can then use the COMSOL Multiphysics particle tracing capabilities to predict particle motion, including rotation, and inertial focusing by applying the developed expressions as user-defined force and moment equations.

Validation and Results

The model was first validated against the established solution for straight channel flow in a 50 µm square cross-section channel. In this case, the equilibrium particle positions are known to be centered on each face of the square and 10 µm away from the walls for a 10 µm diameter particle at a channel Reynolds number of 20.

We then compared the CFD model predictions to experimental measurements for both straight and curved channels that are 50 µm tall, 100 µm wide and 4 cm long. Figure 3 shows experimental and simulation results for a channel Reynolds number of 100 and three Dean numbers: 0, 6 and 9 (the channel is straight when the Dean number is zero). For each case, we show the particle distribution along the channel length collected using fluorescent streak microscopy and the force field calculated for that cross-section with the equilibrium positions (net force = 0) highlighted. The simulation results are in good agreement with experimental measurements for all three cases, and illustrate the dependence of the equilibrium positions on the channel curvature. Figure 4 shows the velocity in the channel and surface tractions on the particle for one channel/particle configuration where the force is dominated by the wall-particle interaction.

The ability to rapidly iterate through design changes in COMSOL Multiphysics and build a comprehensive theory for the operation of such devices will save experimental time as well as guide the design and optimization of our life-saving diagnostic devices. ■